

5th Annual Practical
Applications of NMR
in Industry Conference

SONESTA RESORT HILTON HEAD ISLAND • HILTON HEAD ISLAND, SC



February 20 – 23, 2017

PROGRAM GUIDE



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WELCOME RECEPTION

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You are cordially invited to join the Welcome Reception in the Exhibit Hall on Monday from 6:15 - 8:15 pm. This complimentary reception is the perfect opportunity to casually network with other delegates, exhibitors, sponsors, poster presenters, and speakers in an informal setting. Cocktails and light hors d'oeuvres will be served. **Please join us!**

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CONFERENCE PROCEEDINGS LINK

Please use the link below to access copies of the speaker presentations that have been submitted to date, as well as conference agendas, poster abstracts, speaker information and sponsor and exhibitor websites.

Link	http://cii-resource.com/chi/PANIC-04-03/login.asp
User Name	Your email address
Password	nmr177300 (<i>Please note: passwords are case sensitive</i>)

Following the conference, we will send out the link via email containing updated presentations and/or late submissions. This link will remain active for six weeks after the conference has ended. Please make sure you access the link and save any files you might want prior to that date. If you are looking for a specific set of slides not on the site, please contact the speaker directly for more information. Once the website has been taken down, these files will no longer be available.

If you have not received the updated link two weeks after the close of the meeting, please contact **Pamela Gerardi** in Customer Service at pgerardi@healthtech.com.

MONDAY, FEBRUARY 20

4:30 pm Pre-Conference Registration Open (*Santee Ballroom Foyer*)

6:15 Welcome Reception in the Exhibit Hall with Poster Viewing, Even and Odd Numbered Posters
(*Santee Ballroom E-H*)

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8:15 End of Day

TUESDAY, FEBRUARY 21

(*Santee Ballroom A-D*)

8:15 am Registration & Morning Coffee (*Santee Ballroom Foyer*)

8:45 Chairs' Welcome
Gonzalo Hernandez, Vis Magnetica NMR Consulting
Kristie M. Adams, Dupont

FORENSICS

8:50 Chairperson's Remarks
Torsten Schoenberger, Bundeskriminalamt

9:00 Interactive Datahub to Facilitate Identification of Emerging Synthetic Drugs (ESDs)
Aaron Urbas, Ph.D., NIST

9:30 The Increasing Need for Structure Elucidation Experts in Forensic Drug Analysis
Charlotte Corbett, Ph.D., Senior Forensic Chemist, Special Testing & Research Laboratory, DEA

10:00 Application of NMR Methods for the Resolution of Forensic Cases at the Swedish National Forensic Center
Simon Dunne, Professor, Swedish National Forensic Center

10:30 Coffee Break in the Exhibit Hall with Poster Viewing, Even Numbered Posters
(*Santee Ballroom E-H*)

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POLYMERS

11:20 Chairpersons' Remarks
Jim DeFelippis, The Dow Chemical Company
Michael C. Davis, Bridgestone Americas Center for Research and Technology

11:30 **The Versatility of Liquid State NMR Spectroscopy in Polymer Chemistry and Engineering: An Industrial Perspective**

Ard Kolkman, Ph.D., DSM

12:00 pm **2D Quantitative NMR for Large Molecules**

Patricia Sepulcri, Ph.D., Sanofi Pasteur Marcy L'Etoile

12:30 **Field-Cycling NMR Relaxometry as a Versatile Tool of Molecular Rheology**

Ernst Roessler, Professor, University of Bayreuth

1:00 **Luncheon Presentation: Insight into Reactions, Identification and Quantification**

Kim Colson, Ph.D., Business Development Manager, Bruker BioSpin

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1:45 **Session Break**

2:30 **Introduction to Friday's Validation Workshop**

Torsten Schoenberger, Bundeskriminalamt

PHARMACEUTICALS

2:45 **Chairpersons' Remarks**

John Marino, NIST

Carlos Amezcua, Baxter International, Inc.

2:55 **High-Throughput Analysis of Antibiotics Using Capillary Stop Flow NMR**

David Keire, Ph.D., U.S. FDA

3:25 **Overcoming Challenges with Identification of Ingredients for Counterfeit Drug Investigations**

Charles Pathirana, Ph.D., Bristol-Myers Squibb

3:55 **Water Proton NMR for Noninvasive Pharmaceutical Analysis**

Bruce Yu, Professor, University of Maryland

4:25 **Multi-Attribute Determination Using NMR to Ensure Success**

Michael Jones, Ph.D., Pfizer

4:55 **Light Reception in the Exhibit Hall with Poster Viewing, Odd Numbered Posters (Santee Ballroom E-H)**

5:45 **Transition to Pavilion**

6:00 **Coastal Grill Out Party* (Pavilion)**

**The Coastal Grill Out Party is complimentary to all conference attendees and one guest. RSVP is required. Please see the Registration Desk if you did not RSVP and plan on attending.*

9:00 **End of Day**

WEDNESDAY, FEBRUARY 22

(Santee Ballroom A-D)

8:15 am **Morning Coffee** (*Santee Ballroom Foyer*)

8:45 **Chairs' Welcome**

Gonzalo Hernandez, Vis Magnetica NMR Consulting
Kristie M. Adams, Dupont

STRUCTURE ELUCIDATION AND COMPLEX MIXTURES

8:50 **Chairperson's Remarks**

David Cistola, M.D., Ph.D., Texas Tech Health Sciences Center El Paso

9:00 **CLIP-COSY: Rapid Acquisition of COSY-Type Correlation Spectra with In-Phase Signal Character**

Lukas Kaltschnee, Ph.D., NIH

9:30 **Marine Natural Products as a Challenge for an NMR-Based Structure Elucidation**

Matthias Köck, Ph.D., Alfred-Wegener Institute

10:00 **The NIST Metabolomics Data Quality Initiative: qMet**

Dan Bearden, Ph.D., NIST

10:30 **Coffee Break in the Exhibit Hall with Poster Viewing, Odd Numbered Posters** (*Santee Ballroom E-H*)

PETROLEUM AND PETROCHEMISTRY

11:20 **Chairpersons' Remarks**

Sonia M. Cabral de Menezes, Petrobras R&D Center
Katherine Wu, Albemarle Corporation

11:30 **NMR Spectroscopy and Calculus of the Average Molecular Parameters of Crude Oils and Fractions**

Juan Carlos Poveda Jaramillo, Professor, Universidad Industrial de Santander

12:00 pm **Supporting Development of New Refining Technologies Using Simple and Quick NMR Methodologies**

Ajit Pradhan, Ph.D., Chevron Energy Technology Company

12:30 **Research and Development in Porous Media NMR with Applications for the Oil Industry**

Tito J. Bonagamba, Professor, Universidade de São Paulo

1:00 Luncheon Presentation

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Only 3 Calibrants for IC qHNMR

Charlotte Corbett, Ph.D., Senior Forensic Chemist, Special Testing & Research Laboratory, DEA

Recent Developments with Concepts for Experiment Introduction into JEOL NMR

Ron Crouch, NMR Applications Consultant, JEOL USA, Inc.

The Influence of Data Processing on Results of qNMR Interlaboratory Comparison Study

Takako Suematsu, Ph.D., NMR Application Chemist, Marketing, JEOL USA, Inc.

1:45 Session Break

FOOD AND AGRICULTURE

2:30 Chairperson's Remarks

Adriana Carvalho de Souza, DSM Biotechnology Center

2:40 Rapid and Quantitative Assessment of Early Lipid Oxidation in Food Emulsions During Shelf-Life by Nuclear Magnetic Resonance

Donny Merckx, Unilever

3:10 Investigation of Egg Yolk Lipids with NMR

Svenja Ackermann, Chemical and Veterinary Investigation Office, CVUA Karlsruhe

3:40 Several NMR Applications for the Analysis of Foods and Dietary Supplements

Clark Ridge, Ph.D., U.S. FDA

4:10 Refreshment Break in the Exhibit Hall with Poster Viewing, Even Numbered Posters (Santee Ballroom E-H)

PLANT PRODUCTION/PROBLEM SOLVING

5:05 Chairperson's Remarks

J. Andrew Surface, PPG Industries, Inc.

5:15 NMR Spectroscopy as a Tool for Process Development and Optimization

Erik von Harbou, Professor, University of Kaiserslautern

5:45 Plant Support Using NMR

Sarah Mattler, Ph.D., Exxon Mobil Chemical Company

6:15 Compact NMR Spectroscopy for Sustainable and Flexible Production of High Quality Chemical Products

Simon Kern, BAM

6:45 **Networking Reception in the Exhibit Hall with Poster Viewing, Even and Odd Numbered Posters** (*Santee Ballroom E-H*)

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7:45 **End of Day**

THURSDAY, FEBRUARY 23

(*Santee Ballroom A-D*)

8:15 am **Morning Coffee** (*Santee Ballroom Foyer*)

8:45 **Chairs' Welcome**
Gonzalo Hernandez, Vis Magnetica NMR Consulting
Kristie M. Adams, Dupont

SOLIDS/DNP

8:50 **Chairperson's Remarks**
Michael C. Davis, Bridgestone Americas Center for Research and Technology

9:00 **From Traditional Small Molecules to Novel Liquid Crystal Formulations in Drug Development: A Solid-State NMR Journey**
Anuji Abraham, Ph.D., Bristol-Myers Squibb

9:30 **Dynamic Nuclear Polarization (DNP) Enhanced Solid-State NMR Investigations of Pharmaceuticals**
Yongchao Su, Ph.D., Merck Research Laboratories

10:00 **Structural Investigation of Organic Materials by Solid-State Dynamic Nuclear Polarization Nuclear Magnetic Resonance Spectroscopy**
Stephane Viel, Professor, Aix-Marseille University

10:30 **Coffee Break in the Exhibit Hall with Poster Viewing, Even and Odd Numbered Posters** (*Santee Ballroom E-H*)

LOW-FIELD/BENCHTOP

11:30 **Chairperson's Remarks**
Kathleen Farley, Pfizer, Inc.

11:40 **Nondestructive Materials Testing and Reaction Monitoring with Compact NMR Instruments**
Bernhard Blümich, Professor, RWTH Aachen University

12:10 pm **Advanced Methods in TD-NMR Relaxometry: Applications in Agriculture and Food Products**
Luiz Colnago, Ph.D., EMBRAPA Instrumentação

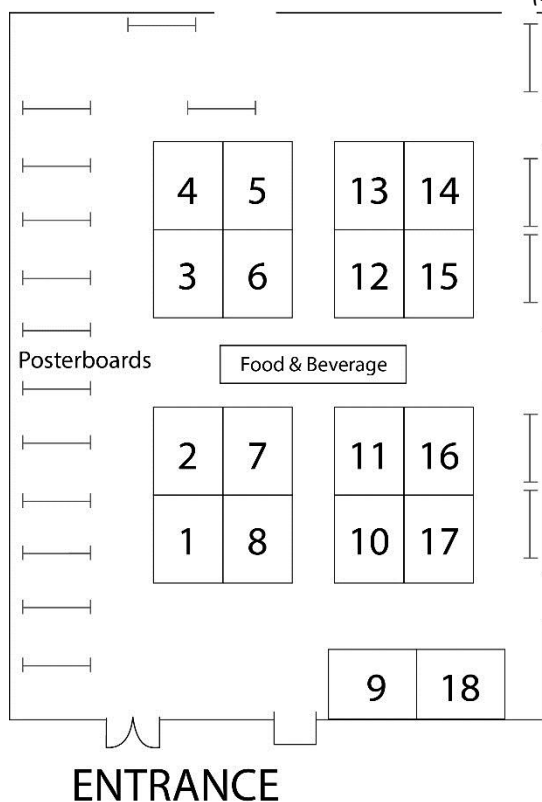
- 12:40** **¹⁹F and ¹H TD-NMR Prospective Applications in Quantitation and Qualitative Analysis for Small and Large Molecule Pharmaceuticals**
Maria Victoria Silva Elipe, Ph.D., Amgen
- 1:10** **Networking Luncheon Hosted by PANIC**
- 1:55** **Session Break**
- 2:40** **Poster Awards & Spectrum Contest Winners Announced**
Poster awards provided by MRC/Wiley

DATA PROCESSING AND ANALYSIS TOOLS

- 2:55** **Chairperson's Remarks**
Kristie M. Adams, Dupont
- 3:05** **Non-Uniform Sampling for All: More Spectral Quality, Less Measurement Time**
Frank Delaglio, Ph.D., IBBR, NIST
- 3:35** **NMR Mixture Analysis Using Machine Learning**
Paul Coote, Ph.D., Harvard Medical School
- 4:05** **Using R to Make Sense of NMR Datasets**
Bryan Hanson, Professor, DePauw University
- 4:35** **Panel Discussion with Speakers**
Moderator: Kristie M. Adams, Dupont
Panelists: Paul Coote, Ph.D., Harvard Medical School
Frank Delaglio, Ph.D., IBBR, NIST
Bryan Hanson, Professor, DePauw University
- 4:55** **End of PANIC 2017**

FLOOR PLAN, EXHIBIT, AND POSTER SCHEDULE

(Santee Ballroom E-H)



COMPANY	BOOTH
Advanced Chemistry Development (ACD/Labs)	5
Aspect AI	14
Bruker BioSpin	3 & 4
Doty Scientific, Inc.	10
HTS-110 Ltd	15
JEOL USA, Inc.	8
Magritek Inc.	11
Mestrelab Research	2
MilliporeSigma	7
Nanalysis	6
New Era Enterprises, Inc.	13
Oxford Instruments	1
Quantum Design	9
Stelar	17
Wako Pure Chemical Industries, Ltd.	12
Wilmad-LabGlass	16

Exhibit and Poster Schedule

Monday:

6:15 - 8:15 pm

Welcome Reception - **Even and Odd Posters** (Hosted by Advanced Chemistry Development (ACD/Labs), Bruker BioSpin, & Mestrelab Research)

Tuesday:

10:30 - 11:20 am

4:55 - 5:45 pm

Coffee Break - **Even Posters** (Sponsored by Oxford Instruments)
 Networking Reception - **Odd Posters**

Wednesday:

10:30 - 11:20 am

4:10 - 5:05 pm

6:45 - 7:45 pm

Coffee Break - **Odd Posters**
 Refreshment Break - **Even Posters**
 Networking Reception – **Even and Odd Posters & Last Chance to Drop Off Your Entry for the Spectrum Contest** (Sponsored by Bruker Biospin)

Thursday:

10:30 - 11:30 am

Coffee Break – **Even and Odd Posters**

Exhibit Hours are subject to change.

SPONSOR & EXHIBITOR COMPANY DESCRIPTIONS

Advanced Chemistry Development (ACD/Labs)

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8 King Street East, Suite 107

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POSTERS

(Santee Ballroom E-H)

Presenting Monday, February 20 – Thursday, February 23

Advanced Chemistry Development, Inc.

1. Steve Coombes; John Nightingale; Azalea Micottis; Albert Van Wyk; Peter Russel; Stephane Albrecht; and Dimitris Argyropoulos: *Impurity Lifecycle Management: Visualising a Vast Array of NMR and Other Analytical Data*

Baxter International, Inc.

2. Jürgen Siekmann; Richard Scheinecker; Zhenqing Zhang; Mikhail V. Gerasimov; Christina M. Szabo; Paul Kosma; and G. Joseph Ray: *Reaction of Oxidized Polysialic Acid and a Diaminoxy Linker: Characterization and Process Optimization Using Nuclear Magnetic Resonance Spectroscopy*

Bundesanstalt für Materialforschung und -prüfung (BAM)

3. Klaus Rademann; Michael Maiwald; and Klas Meyer: *Quantitative NMR Spectroscopy for Gas Metrology - Applications in Liquefied Petroleum Gases*

Case Western Reserve University

4. Fengchao Zhang and Cheng Chen: *Broadband Quantitative NQR Analysis of Medicines and Nutritional Supplements*

Colorado State University

5. Claudia Boot; Kim Colson; Torsten Schoenberger; Kristie Adams; and Kaylen Obray: *NMR Validation: Significance, Implementation, and Awareness*

Dow Chemical Company

6. Tianlan Zhang; Wenqin (Sunny) Wang; and Jun Qi: *Investigating the Composition, Functionality, and Composition-Viscosity Relationship of Multi-Functional Acrylate, a Key Material in UV Curable Coatings*

DSM Biotechnology Center

7. Joep van Rijn; Paul Groen; and Adriana Carvalho de Souza: *Robust and Reliable Quantification of Phospholipids in Edible Oils*

ESPCI Paris

8. J.-C. Ameline; A. Chateauminois; R. Gautier; H. Montes; G. Lang; L. Le Polles; N. Lequeux; C. Roiland; J.-B. d'Espinose de Lacaillerie; and Romain Dubourget: *Structural Health Monitoring Using Nuclear Quadrupole Resonance as a Stress Gauge*

Fine Instrument Technology (FIT)

9. D.M. Consalter; D.W. Flores; S.P. Azevedo; T.B. Moraes; L.A. Colnago; and Andre S. Carvalho: *Using Low Field NMR for Process Control in Palm Oil Industry*
10. Douglas Flores; Andre S. Carvalho; Daniela Kharfan; Luiz Alberto Colnago; and Daniel M. Consalter: *TD-NMR Applied to Citrus Process Control: Method Evaluation*

Food and Drug Administration

11. Sharadrao Patil: *Independent Assessment of 2D DOSY NMR and DLS in Measuring Diffusion Coefficients of Insulin Formulations: Implication for Particle Size Distribution Methods*

Hochschule Bonn-Rhein-Sieg

12. Patrick Jonas; Bernd W.K. Diehl; and Elina Zailer: *Alternative Method for Relaxation Time Determination*

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13. Junko Hosoe; Naoki Sugimoto; Yuko Yamada; Toru Miura; Hiroki Suzuki; Takao Katsuhara; Yasushi Igarashi; Hiroaki Nishimura; Yuichi Kikuchi; Tadatoshi Yamashita; Yukihiko Goda; and Takako Suematsu: *Application of Quantitative ¹H NMR to Hygroscopic Reagents*

Louisiana State University

14. Thilini Ukwathhage; Megan Macnaughtan; and Abigael C. Songok: *Towards the Three Dimensional Structure of Chlamydia trachomatis Protein Scc4 and Its Binding Interface with Scc1 by Solution NMR Spectroscopy*

Millipore Sigma

15. Romana Rigger; Christine Hellriegel; Robert Sauer Moser; Markus Obkircher; and Alexander Rueck: *Development of Certified Reference Materials (CRM) for ¹H, ³¹P and ¹⁹F Quantitative NMR*

National Institute of Standards and Technology

16. Luke W. Arbogast; Robert G. Brinson; John P. Marino; and Frank Delaglio: *Non-Uniform Sampling for All: More Spectral Quality, Less Measurement Time*
17. Katrice A. Lippa; Anthony Windust; Alexander Rueck; Markus Obkircher; and Michael A. Nelson: *Achieving Traceability in Practice: Development of NIST PS1 Primary Standard for Quantitative NMR (Benzoic Acid)*
18. Ryan Nieuwendaal: *Critical Experimental Details of ¹H Spin Diffusion NMR Towards Measuring Miscibility and Domain Sizes in Polymer Blends*

National Institutes of Health, National Institute of Diabetes and Digestive and Kidney Diseases

19. Jonas Kind; Martin Leyendecker; Christina M. Thiele; and Lukas Kaltschnee: *Monitoring a Four-State Photoisomerization Process via In Situ Irradiation NMR Spectroscopy*

National Research Council Canada

20. Mohammad Raza; Jeremy Melanson; Maohui Chen; Martin Couillard; Zygmunt J. Jakubek; Tianyang Leng; Linda J. Johnston; and Andreas Brinkmann: *Quantitative Solid-State NMR Applications in Chemical Metrology*

Ohio University

21. Peter B. Harrington; Steven F. Baugh; and Xinyi Wang: *Comparative Study of NMR Spectroscopy Profiling for the Characterization of Cannabis*

Pfizer, Inc.

22. Forrest Beaulieu; Brian Chekal; and Heather Frericks Schmidt: *Monitoring Levels of Crystallinity in Milled APIs Using Low Field Benchtop NMR*
23. John Braganza; Jason Ewanicki; Paul Richardson; and Wei Wang: *Closed Loop Reaction Monitoring Using Benchtop ¹⁹F NMR at 41 MHz*

Politecnico di Bari

24. Piero Mastrorilli; Mario Latronico; Nicola Intini; Pasquale Scapicchio; Antonino Rizzuti; and Vito Gallo: *Validation Criteria for Simultaneous Multi Component Quantitative NMR Analysis and NMR Fingerprinting Methods*
25. Vito Gallo; Nicola Intini; Mario Latronico; and Piero Mastrorilli: *NMR as a Tool for Measuring the Storage Potential of Table Grapes*

Technischen Universität Kaiserslautern

26. Erik von Harbou; Hans Hasse; and Richard Behrens: *Quantitative NMR Spectroscopic Study of Highly Dilute Key Components in Complex Reactive Mixtures: CO₂ in Aqueous Amine Solutions*

Texas Tech University Health Sciences Center, El Paso

27. Vipulkumar Patel; Sneha Deodhar; Ina Mishra; and David P. Cistola: *Benchtop NMR Relaxometry in Clinical Diagnostics: Whole Human Blood*

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